Modeling switching in STM molecular junctions

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A broadly observed phenomenon in experiments on molecular junctions is time dependent switching of the tunneling current[1-5]. In many cases such behavior involves different current states which are attributed to the transfer of single atoms or functional groups in a molecule between different stable configurations. We describe here the investigation of the current switching observed in a molecular junction formed by a PTCDA molecule between an STM tip and an Ag(111) surface, which is believed to be due to the carboxylic oxygen atom switching between the surface and the tip[6]. We use a generalized version of a model developed in 1997 by Gao et al.[7] to investigate the results observed in these experiments. The distribution of the switching events measured in the experiments shows a power law dependence for small positive bias voltages, whereas for negative voltages it shows a constant behavior. Compared to Gao's model, which can only describe the rapid increase of the switching events at a certain onset voltage, our extended model can be used to characterize the whole distribution relating the different behavior to the changes in the potential by the applied bias.

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